

Methanesulfonic acid
75-75-2 | DTXSID4026422

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.933

Global applicability domain: Inside

Local applicability domain index: 4.68e-01

Confidence level: 3.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dimethyl sulfoxide</div> <div>Measured: -1.35</div> <div>Predicted: -1.15</div>	<div>Image not found</div> <div>Methanesulfonyl fluoride</div> <div>Measured: 0.55</div> <div>Predicted: 2.61e-01</div>	<div>Image not found</div> <div>Dimethyl sulfone</div> <div>Measured: -1.41</div> <div>Predicted: -1.07</div>
<div>Image not found</div> <div>Fosetyl</div> <div>Measured: -2.70</div> <div>Predicted: -2.12</div>	<div>Image not found</div> <div>3-Chloropropionitrile</div> <div>Measured: 0.18</div> <div>Predicted: 3.72e-01</div>	